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FINAL TECHNICAL REPORT ON WORK SUPPORTED BY ONT  
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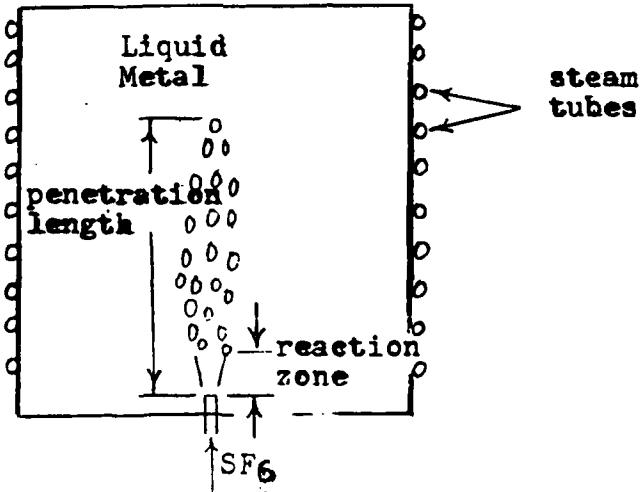
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INTRODUCTION, BACKGROUND

This report summarizes the research conducted during my stay at NOSC as an ONT postdoctoral fellow. The basic motivation for this work was to better understand the process of liquid metal combustion in Stored Chemical Energy Propulsion Systems (SCEPS) of interest to the NAVY as underwater propulsion systems. The chemical system of greatest current interest is the Li-SF<sub>6</sub> system. A schematic diagram of a typical SCEPS reactor configuration

is shown below:



Here a jet of gaseous SF<sub>6</sub> is introduced into a container of molten lithium

which serves as both a reactor and a boiler. Reaction is presumably completed quite near the injector, the remaining gaseous portion of the jet consisting largely of condensing lithium vapor formed by the intense heat of reaction. An important quantity to be predicted is the penetration length, the length of the gaseous jet in the boiler-reactor. In the design of a boiler-reactor, the penetration length would be less than the reactor length in order to avoid undesired effects associated with the build-up of vapor in the reactor. Other predictions of interest are temperature fields, velocity fields, and the distribution and composition of the gas and liquid phases.

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The typical SCEPS combustion process is possessed of a number of characteristics which render a complete mathematical description extremely difficult. These include:

1. Extreme temperatures → importance of radiation effects
2. Formation of immiscible liquid/solid products → stratification effects, etc.
3. Inherent difficulty of the process of the impingement of a gas jet into a liquid → basic flow regimes not well understood

The basic approach to the mathematical modelling of liquid metal combustion in SCEPS reactors to date has been based on some form of locally homogeneous flow (LHF) model. Here the two-phase flow is treated as an effectively single-phase flow, the principle assumption being that at each point in the flow, the velocity and temperature of the gas and liquid phases are the same and phase and chemical reaction equilibrium are attained. The thermodynamic and transport properties are functions of the amount of gas relative to liquid and the transport equations assume the same form as for single-phase flows; these equations can be solved using modifications of existing numerical routines.

LHF models would be expected to be good for describing the SCEPS combustion process beyond the point at which the gas jet breaks up into numerous small bubbles. However, it is probably not adequate to describe the details of the near-injector region where one has:

1. a reaction zone
2. a more or less continuous jet of gas
3. complicated flow phenomena such as reverse shocks

Ideally, a mathematical model of the SCEPS combustion process would include separate equations for each phase and would treat the physicochemical phenomena discussed above. Models which include separate equations for each phase are generally known as separated flow models; this type of model has been applied in a limited way to simpler processes such as sprays of various types. The components of a separated flow model of the SCEPS combustion process would include:

1. Quantitative details of the process by which drops and bubbles are formed (flow regimes)
2. Transport equations for the gas and liquid phases
3. Expressions for the rates of interphase transport of chemical species, energy, momentum
4. Expressions for the rates of the various chemical reactions involved

Typically, the liquid droplets might be tracked as they move through the gas phase, with the interphase transport rates appearing as source terms in the gas phase transport equations.

The ultimate goal of the present work is to understand better the flow

regimes involved in the interaction of gas jets with liquids, including the effects of such phenomena as gas assimilation, heat transfer, energetic reaction, formation of immiscible phases, etc..

The present work may be divided into two main parts:

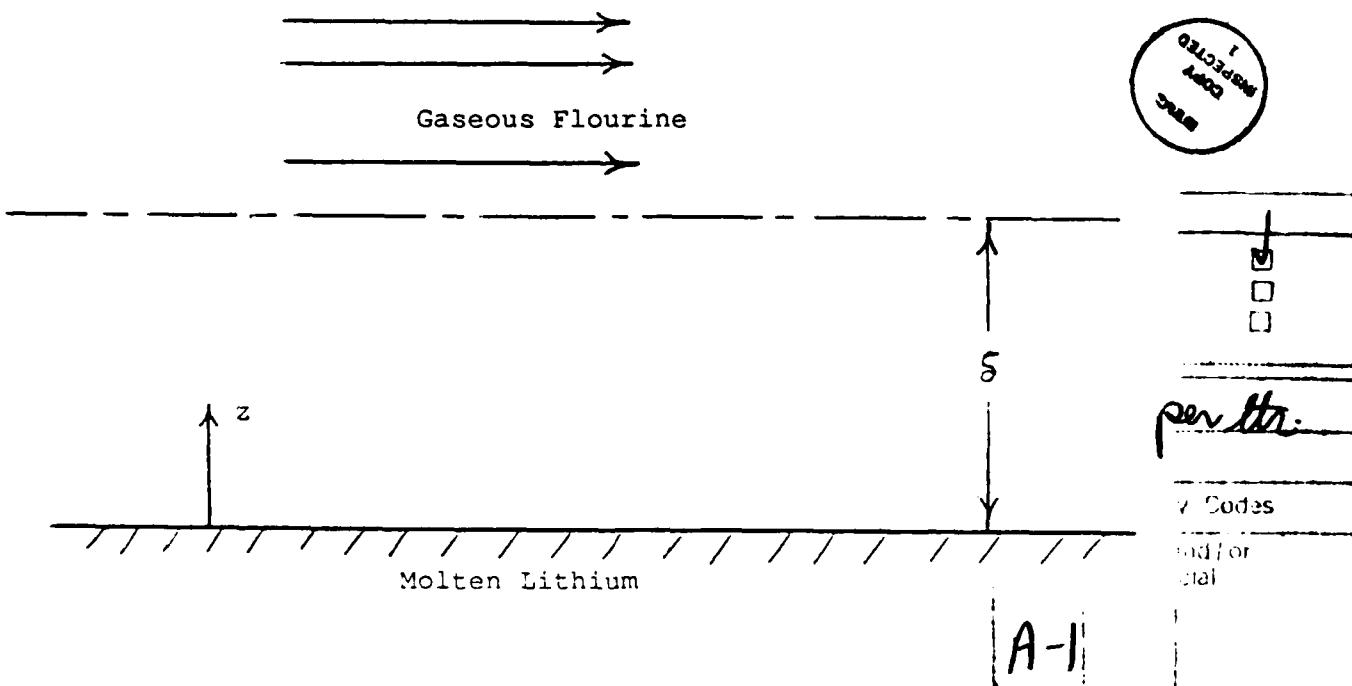
1. Mathematical modelling of liquid metal flames
2. Study of the flow regimes involved in the interaction of gas jets with liquids
  - (a) literature review
  - (b) experimental

#### MATHEMATICAL MODELLING OF LIQUID METAL FLAMES

The problem is considered where a stream of flourine gas interacts with a pool of molten lithium at a planar interface. This problem is considered for several reasons: (1) it is somewhat simpler than the corresponding problem involving the Li-SF<sub>6</sub> system, but possesses many of the same features; (2) it

may be regarded as a component of a separated flow model of a SCEPS combustion process; (3) it would probably be desirable to carry out experiments on liquid metal combustion in laboratory devices in which the geometry is simple and the mass transfer rates are well-defined (rotating disk, stagnation point flow, etc.) to which this problem would be relevant.

Here follows a schematic diagram of the problem to be considered:



Here  $\delta$  is the thickness of the mass transfer boundary layer, or "film thickness", which will be discussed further in the next paragraph.

In order to simplify the mathematical description of the problem, a number of simplifying assumptions are made:

1. all species mass diffusivities are equal
2. Lewis number,  $\frac{\lambda}{\rho C_p D} = 1$
3. constant gas phase properties evaluated at interface temperature
4. all liquid-phase heat capacities and heats of vaporization equal
5. at the gas-liquid interface, a single phase containing both lithium and the product lithium fluoride exists. Separation into a fuel-rich and product-rich phase then presumably occurs at some distance below the interface.
6. Gas-liquid thermodynamic equilibrium holds at the interface; equilibrium is treated by means of Raoult's law
7. Convective mass transfer is treated by means of the stagnant film model. That is, a hypothetical stagnant film of thickness  $\delta$  is presumed to exist adjacent to the gas-liquid interface, within which mass transfer is by diffusion and by convection resulting from the interphase mass transfer of fuel and product species.
8. The condition of chemical reaction equilibrium holds everywhere in the gas phase.

Under these assumptions, the governing equations take the following form:

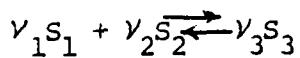
1. equations for reaction-invariant variables

$$\rho v \frac{db}{dz} = \rho D \frac{d^2 b}{dz^2}$$

with

$$b_1 \equiv \frac{y_2 - \frac{y_1}{v_1} y_1}{b_{ls} - \frac{\dot{m}_2}{\rho_s v_s}} \quad b_2 \equiv \frac{\Delta H_{r,2} y_2 + C_p T}{\Delta H_{r,2} (y_{20} - \frac{\dot{m}_2}{\rho_s v_s}) + Q}$$

Here the reaction considered ( $\text{Li} + \text{F} \rightarrow \text{LiF}$ ) is written as:



and

$$S_i \equiv \text{species } i \quad (S_1 \equiv \text{F}, S_2 \equiv \text{Li}, S_3 \equiv \text{LiF})$$

$y_i$  = mass fraction of species i  
 $c_p$  = gas-phase heat capacity  
 $b_{ls}$  = interfacial value of  $b_1$   
 $\dot{m}_{20}$  = interfacial mass flux of Li  
 $\rho_{ss}^v$  = net interfacial mass flux  
 $T$  = temperature  
 $\Delta H_{r,2}$  = heat of reaction per unit mass Li  
 $\Omega = \Delta H_{vap.} + c_{p,1}(T_s - T_{l,b})$   
 $\Delta H_{vap.}$  = heat of vaporization  
 $c_{p,l}$  = liquid-phase heat capacity  
 $T_s$  = temperature at interface  
 $T_{l,b}$  = bulk liquid temperature

## 2. condition of chemical reaction equilibrium

$$\frac{y_3}{y_1 y_2} = K(T)$$

with

$y_i$  = mole fraction, species i

$$= \frac{y_i / M_i}{\sum_j y_j / M_j}$$

$K(T)$  = equilibrium constant (function of temperature)

$$3. \quad \sum_j y_j = 1$$

The boundary conditions employed are the following

1. far-field temperature, concentrations
2. heat, mass-flux conditions at interface

### 3. temperature, concentrations at interface

Subject to the assumptions employed, the governing equations for the reaction-invariant variables may be solved analytically to yield

$$b = (b_s - 1) + (b_{\infty} - b_s + 1) \exp \left[ \frac{\rho v}{pD} (z - S) \right]$$

The values of the reaction invariant variables at the interface,  $b_s$ , are determined by applying the conditions of chemical reaction and phase equilibrium at the interface. The values of the species mass fractions and temperature at any location within the mass transfer boundary layer are then determined by applying simultaneously, the above expression for the invariants, the condition of reaction equilibrium, and  $\sum_j y_j = 1$ .

At present, calculations have been carried out as discussed above for one set of specified boundary conditions. Some results of interest are:

1. mass fluxes at interface
2. mass fractions and temperature as functions of position
3. maximum temperature and position of maximum temperature

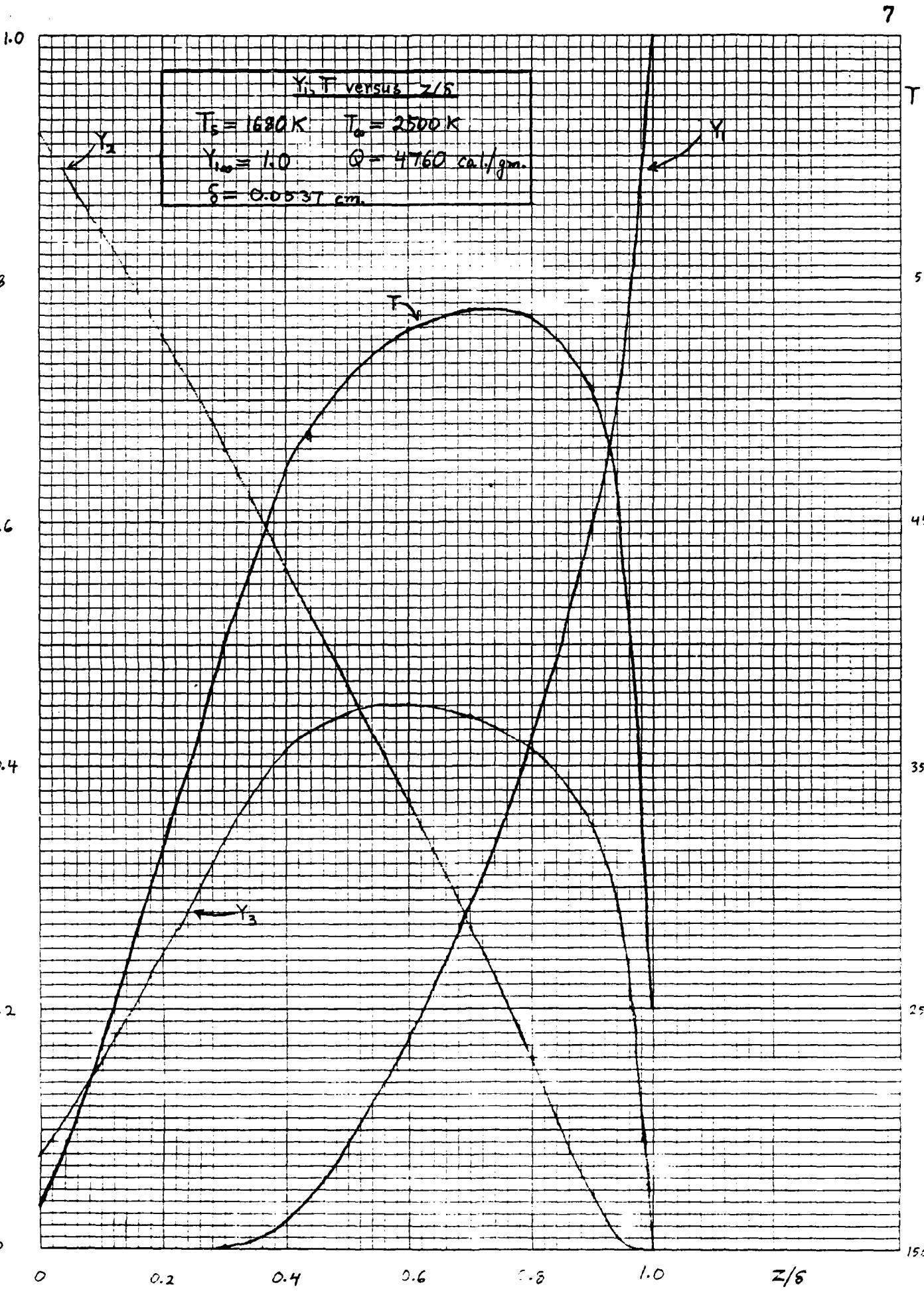
Shown below is a plot of the mass fractions and temperature as functions of position along with a listing of the parameters employed in the calculations.

The maximum temperature obtained from these calculations is about 5000 K. The equations for the mass fractions and temperature were solved easily using a standard IMSL subroutine. In the future, it would be of interest to carry out the following work related to the above:

1. Further calculations similar to the above
  - (a) calculations employing more accurate thermodynamic equilibrium relations
  - (b) calculations employing more accurate transport properties
  - (c) calculations for other values of the boundary parameters
  - (d) calculations for Li-SF<sub>6</sub>, other systems
  - (e) calculations employing other assumed mechanisms of product condensation
  - (f) similar calculations for systems in which mass/energy transfer can be accounted for more rigorously.
2. Experiments on liquid metal combustion in laboratory devices in which mass/energy transfer can be conveniently and accurately accounted for

### INTERACTION OF GAS JETS WITH LIQUIDS

The problem is considered here where a jet of gas enters through a round nozzle into the bottom of a tank of liquid which may or may not react with the gas. The basic methodology employed consists of carrying out a literature review and conducting experiments. The basic goal is to understand the flow regimes arising in the interaction of gas jets with liquids including the effects of such phenomena as exothermic reaction and



liquid vaporization/recondensation and ultimately apply this knowledge to the development of improved models of SCEPS reactors. The description of the gas/liquid flow regime would constitute an essential part of a separated flow model of a SCEPS reactor. With regard to modelling of SCEPS reactors, the primary emphasis would be on the near-nozzle region, where LHF models are believed to be most inadequate. It may be possible to identify and characterize flow regimes especially troublesome/advantageous in the operation of SCEPS reactors.

A large number of studies, mostly experimental, have considered the bubbling of gases through liquids. However, relatively little effort has been focused upon flow regimes occurring at very high gas flow rates, which are of greatest interest here. The greatest amount of literature relevant to flow regimes occurring during high rates of gas injection into liquids has appeared relating to the processing of molten metals by gas injection and to "impingement wastage" (the failure of adjacent tubes following rupture of a steam tube cooled by a liquid metal). Much of the information relating to metals processing has appeared in the Soviet literature and most of the literature relating to impingement wastage is connected with the nuclear power industry.

As background, here follows a brief description of the flow regimes described in the literature for the interaction of non-reactive gas jets with liquids.

1. Bubbling
2. Unstable Bubbles
  - (a) bubble growth is from a gas neck at the orifice
  - (b) The A→B transition is possibly connected with the transition to turbulence in the nozzle
3. Unstable Jet (transition)
  - (a) continuous jet whose boundaries pulsate, or string of large connected unstable bubbles originating from gas neck at orifice
  - (b) The B→C transition occurs at approximately the sonic velocity
  - (c) occasional interruption by "reverse shocks"
  - (d) stable gas residual at orifice postulated to be the first shock cell in the underexpanded jet
4. Reverse Shock
  - (a) Frequency of reverse shocks decreases and becomes more random
  - (b) Reverse shock may be due to obstruction of the flow by entrained liquid which results in a gas bubble which subsequently "bursts"

Regarding the effect of gas assimilation on flow regimes, it has been reported in the Soviet literature that in the limit of highly assimilable gases, only two flow regimes exist; a pulsative regime and a pure jet regime (no reverse shocks) in both of which the gaseous portion of the jet disappears close to the nozzle. Heat transfer to a cold gas jet from a hot liquid is believed to suppress severance of the gas column near the nozzle; heat release and an increase in number of moles due to reaction are believed to give rise to similar effects. In at least one study (Cho and Armstrong, Argonne) bubble formation at the nozzle was observed at very high flow rates (underexpanded jet) in the HCl-aqueous NH<sub>3</sub> system; such behavior

may be connected with the vaporization/recondensation of NH<sub>3</sub>. Experiments of

Parnell et.al. at NOSC have indicated that during injection of underexpanded jets of SF<sub>6</sub> gas into molten Lithium, the gaseous portion of the flow may exist as some sort of a pulsating jet.

Some preliminary experimental results were obtained for the air-water and CO<sub>2</sub>-aqueous NaOH systems. The tank containing liquid was made of

plexiglass and was one foot by one foot by two feet in dimension; the gas entered the bottom of the tank through a round nozzle one millimeter in diameter. Flow visualization studies were carried out using high-speed motion pictures shot at 4000-8000 frames per second. The goal of this experimental study was to obtain basic information, via flow visualization, on the effect of chemical reaction and associated effects on the overall flow regimes in gas injection into liquids. In the future, it would be desirable to continue this experimental study.